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PASSWORD:

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Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
         SEP 09
                 CA/CAplus records now contain indexing from 1907 to the
                 present
NEWS
        AUG 05
                 New pricing for EUROPATFULL and PCTFULL effective
                 August 1, 2003
        AUG 13
NEWS
                 Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 6
        AUG 18
                 Data available for download as a PDF in RDISCLOSURE
NEWS
     7
        AUG 18
                 Simultaneous left and right truncation added to PASCAL
NEWS 8
                 FROSTI and KOSMET enhanced with Simultaneous Left and Righ
        AUG 18
                 Truncation
NEWS 9
        AUG 18
                 Simultaneous left and right truncation added to ANABSTR
NEWS 10
        SEP 22
                 DIPPR file reloaded
        DEC 08
NEWS 11
                 INPADOC: Legal Status data reloaded
NEWS 12
        SEP 29
                 DISSABS now available on STN
NEWS 13
        OCT 10
                 PCTFULL: Two new display fields added
        OCT 21
NEWS 14
                 BIOSIS file reloaded and enhanced
        OCT 28
NEWS 15
                 BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16
        NOV 24
                 MSDS-CCOHS file reloaded
        DEC 08
NEWS 17
                 CABA reloaded with left truncation
NEWS 18
        DEC 08
                 IMS file names changed
NEWS 19
        DEC 09
                 Experimental property data collected by CAS now available
                 in REGISTRY
NEWS 20
        DEC 09
                 STN Entry Date available for display in REGISTRY and CA/CAplus
             NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT
NEWS EXPRESS
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
              STN Operating Hours Plus Help Desk Availability
NEWS HOURS
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
              CAS World Wide Web Site (general information)
NEWS WWW
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\*ENCOMPPAT2 - EnCompass Patent File 1964-Present (Non-Supporters)

\* The files listed above are temporarily unavailable.

FILE 'HOME' ENTERED AT 11:48:08 ON 14 DEC 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:48:17 ON 14 DEC 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 12 DEC 2003 HIGHEST RN 626603-92-7 DICTIONARY FILE UPDATES: 12 DEC 2003 HIGHEST RN 626603-92-7

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d
ENTER NAME OF ITEM TO BE DISPLAYED OR (?):
Uploading
'UPLOAD' IS NOT VALID HERE

For an explanation, enter "HELP DISPLAY".

=> 09893858.str

0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

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The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

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0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

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The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d

ENTER NAME OF ITEM TO BE DISPLAYED OR (?):end

=>

Uploading 09893858.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 11:49:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7824 TO ITERATE

100.0% PROCESSED 7824 ITERATIONS

48 ANSWERS

SEARCH TIME: 00.00.01

L2 48 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 148.55 148.76

FILE 'CAPLUS' ENTERED AT 11:49:19 ON 14 DEC 2003

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FILE COVERS 1907 - 14 Dec 2003 VOL 139 ISS 25 FILE LAST UPDATED: 12 Dec 2003 (20031212/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L3 68 L2

=> s l3 and acrylonitrile

83204 ACRYLONITRILE

937 ACRYLONITRILES

83461 ACRYLONITRILE

(ACRYLONITRILE OR ACRYLONITRILES)

L4 39 L3 AND ACRYLONITRILE

=> s 14 and dinitrile

1821 DINITRILE

1291 DINITRILES

2645 DINITRILE

(DINITRILE OR DINITRILES)

L5 0 L4 AND DINITRILE

=> d ibib abs hitstr tot 14

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L4 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN ACCESSION NUMBER: 2003:532626 CAPLUS DOCUMENT NUMBER: 139:86730
                                                                                                                    2003:532626 CAPLUS
139:86730
Preparation of a polycarboxylic acid mixture containing mainly 1,3,6-hexanetricarboxylic acid Date, Hideki: Shimoda, Teruyoshi Asshi Kasai Kabasi Kabasi Kabasi Kasai Kabasi Kab
    INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:
   DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                       KIND DATE
PATENT NO. KIND DATE

WO 2003055836 Al 20030710 WO 2002-JP13808 20021227

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, IU, LV, MA, MD, MG, MK, MN, MR, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GA, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO:

JP 2001-397451 A 20011227

AB This document discloses a polycarboxylic acid mixt having a 1,3,6-hexanetricarboxylic acid (I) content of 80 wt.% or higher, a chromaticness index a of -2.0 to 2.0, a chromaticness index b of -2.0 to 3.0, and a nitrogen content of 5,000 wt.ppm or lower. The above mixt.
                          PATENT NO.
                                                                                                                                                                                                        APPLICATION NO. DATE
                          obtained by hydrolysis of a mixt. contg. mainly 1,3,6-tricyanohexane. I is useful as a hardener for compds. contg. epoxy functions and is used in
                         1772-25-4P, 1,3,6-Tricyanohexane
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant
   IT
   οr
                          (prepn. of polycarboxylic acid mixt. contg. mainly 1,3,6-
hexanetricarboxylic acid as hardener for epoxy resins)
1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)
   NC-CH2-CH2-CH-(CH2)3-CN
   REFERENCE COUNT:
                                                                                                                                                  THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
    FORMAT
 L4 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
139:68954
TITLE:
Acid from 1,3,6-tricyanohexane as byproducts of electroreduction of acrylonitrile
Ubutame, Takuji: Shimoda, Akiyoshi
Asahi Kasei Corporation, Japan
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
FAMILY ACC. NUM. COUNT:
FAMILY ACC. NUM. COUNT:
1
                                                                                                                                                                                                                                                                                                                                                                                                                                L4 ANSWER 3 OF 39
ACCESSION NUMBER:
DOCUMENT NUMBER:
139:68953
Preparation of colorless 1,3,6-hexanetricarboxylic acid from 1,3,6-tricyanohexane as byproducts of electroreduction of acrylonitrile
Shimoda, Akiyoshi; Ishida, Hiroshi
Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
Patent
                                                                                                                                                                                                                                                                                                                                                                                                                                  DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     Patent
Japanese
   FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                          PATENT NO.
                                                                                                      KIND DATE
                                                                                                                                                                                                       APPLICATION NO. DATE
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      APPLICATION NO. DATE
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      KIND DATE
 PATENT NO. KIND DATE APPLICATION NO. DATE

JP 2003192631 A2 20030709 JP 2001-397453 20011227

PRIORITY APPIN. INFO.: JP 2001-397453 20011227

AB 1,3,6-Hexanetricarboxylic acid (1) and/or its salts are prepd. by (A) hydrolysis of crude 1,3,6-tricyanohexane (II) obtained by electroredn. of CH3CN and (B) crystn. Thus, a mixt. contg. II 93.3, 3-cyanomethyl-1,5-dicyanopentane 5.8, and adiponitrile 0.9% was hydrolyzed with NaOH, neutralized, water added, and cooled to 3-10.degree. to give 73.9% I having purity of 99.6% and L value of 98.9%.

IT 1772-25-4F, 1,3,6-Tricyanohexane

RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant of
                                                                                                                                                                                                                                                                                                                                                                                                                                 JP 2003192630 A2 20030709 JP 2001-397452 20011227
PRIORITY APPLN. INFO:: JP 2001-397452 20011227
AB 1,3,6-Hexametricarboxylic acid (I) and/or its salts are prepd. by (A) hydrolysis of crude 1,3,6-tricyanohexane (II) obtained by electroredn. of CH3CN and (B) treatment of the reaction mixts. with oxidizing agents. Thus, a mixt. contg. II 93.3, 3-cyanomethyl-1,5-dicyanopentane 5.8, and adiponitrile 0.9% was hydrolyzed with NaOH to give pale brown I, which
                                                                                                                                                                                                                                                                                                                                                                                                                                                        dissolved in water and treated with ozone for bleaching.
1772-25-4P, 1, 3,6-Tricyanohexane
RE: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant
                         (crystn. of hexanetricarboxylic acid prepd. from tricyanohexane as
byproducts of electroredn. of acrylonitrile)
1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)
                                                                                                                                                                                                                                                                                                                                                                                                                                                        reagent)
(03 bleaching of hexanetricarboxylic acid prepd. from tricyanohexane
                                                                                                                                                                                                                                                                                                                                                                                                                                                                       byproducts of electroredn. of acrylonitrile) 2-25-4 CAPLUS
                                                                                                                                                                                                                                                                                                                                                                                                                                                        1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)
  NC-CH2-CH2-CH-(CH2)3-CN
                                                                                                                                                                                                                                                                                                                                                                                                                                 NC-CH2-CH2-CH-(CH2)3-CN
```

L4 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN

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L4 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:510101 CAPLUS
DOCUMENT NUMBER: 139:68960
TITLE: Less-colored trinitrile mixtures and their
preparation
                                                                                        by electrolytic reduction of acrylonitrile
Shimoda, Akiyoshi; Ishida, Hiroshi
Asahi Kasei Corporation, Japan
Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
Patent
Japanese
 INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:
 DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                    PATENT NO.
                                                                                  KIND DATE
                                                                                                                                                                 APPLICATION NO. DATE
JP 2003183239 A2 20030703 JP 2001-389826 20011221
PRIORITY APPLN. INFO.: JP 2001-389826 20011221
AB Less-colored trinitrile mixts., which show content of trinitrile compds.
.gtoreq.85%, content of adiponitrile (I) .ltoreq.10%, L value
(brightness)
of 0.10 g/mL diethylene glycol di-Me ether soln. .gtoreq.98, and a and b values (chromaticness indexes) -1.0-1.0 and -1.0-2.0, resp., are prepd.
                   (1) electrolytic redn. of acrylonitrile in the presence of electrolytes, (2) removal of I and components having b.p. higher than
                 electrolytes, (2) removal of I and components having b.p. higher than of trinitrile compds. from the reaction product mainly contg. I so that content of I is .1toreq.10% and content of trinitrile compds. is .gtoreq.85%, and (3) treatment of the products with solid adsorbents and/or oxidizing agents. Thus, a mixt. contg. 1,3.6-tricyanohexane (II) 93.3, 3-cyanomethyl-1,5-dicyanopentane 5.8, and I 0.9% (L value 99.8, a value -0.20, b value 0.11, and APRA .ltoreq.100) was obtained by the above method. II is useful as a material for 4-aminomethyl-1,8-diaminooctane, 1,3.6-hexanetricarboxylic acid, etc. 1772-25-49, 1,3.6-Tricyanohexane RL: IMF (Industrial manufacture): PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of less-colored trinitrile mixts. by electrolytic redn. of earylontirle and removal of adiponitrile) 1772-25-4 CAPLUS
 |
NC-CH2-CH2-CH-(CH2)3-CN
```

```
ANSWER 5 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
NC-CH2-CH2-
                CH- (CH2) 3-CN
REFERENCE COUNT:
                                       THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT
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```
L4 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:172114 CAPLUS
DOCUMENT NUMBER: 136:215533
Method for an enzymatic reaction of compounds having at least one nitrile function and/or at least one anide function
INVENTOR(S): Hauer, Bernhard; Pressler, Uwe: Ress-Loeschke,
                                                                                                                              Syldatk, Christoph; Christian, Hans-juergen;
      Pietzsch,
                                                                                                                             Markus
Basf Aktiengesellschaft, Germany
PCT Int. Appl., 49 pp.
CODEN: PIXXD2
      PATENT ASSIGNEE(S):
SOURCE:
    DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                               Patent
                           PATENT NO.
                                                                                                              KIND DATE
                                                                                                                                                                                                                   APPLICATION NO. DATE
WO 2002018612 Al 20020307 WO 2001-EP10025 20010830
W: AE, AG, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MZ, NZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VM, YU, 2A, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, MA, TI, BE, CH, CY, DE, DK, ES, FT, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BZ, CT, CG, CM, GA, GM, GQ, GW, ML, MG, NE, SM, TD, TG
DE 10042835 Al 20020314 DE 2000-10042835 20000830
AU 2001091811 AS 20020313 AU 2001-91811 20010830
EF 1315824 Al 20030604 EF 2001-931893 20010830
AR: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, FRIORITY APPLIN. INFO:

DE 2000-10042835 A 20000830

OTHER SOURCE(S):

CASREACT 136:215533
AB The invention relates to the enzymic reaction of compds. having at least one mitrile function and/or at least one mide function with at least one microorganism and/or at least one mide function with at least one microorganism and/or at least one nitrile hydratase-amidase complex isolated from Rhodococcus erythropolis DSM 13475 and Rhodococcus erythropolis DSM 13476. Thus, free cells of
                                                                                                                                         20020307
                            WO 2002018612
                                                                                                                  A1
                                                                                                                                                                                                                   WO 2001-EP10025 20010830
 isolated from Rhodococcus erythropolis DSM 13002, Rhodococcus erythropolis
DSM 13475 and Rhodococcus erythropolis DSM 13476. Thus, free cells of Rhodococcus erythropolis DSM 13072 reduced - 90 mM propanenitrile to produce propanamide in 15 min. The resulting propanamide was then slowly deamidated to produce propanoic acid.

IT 1772-25-4, 1,3,6-Hexanetricarbonitrile
RL: BSU (Biological study, unclassified); BIOL (Biological study) (enzymic redn. and deamidation with Rhodococcus nitrile hydratase and amidase)
RN 1772-25-4 CAPLUS
CN 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)
  L4 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN ACCESSION NUMBER: 2002:31043 CAPLUS DOCUMENT NUMBER: 136:71544
TITLE: Process 6
                                                                                                                            Process for the preparation of 1,3,6-
hexanetricarbonitrile
```

```
Schelhaas, Michael; Jautelat, Manfred
Bayer Aktiengesellschaft, Germany
Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
    INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:
     DOCUMENT TYPE:
                                                                                                                                                  Patent
    LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                               PATENT NO.
                                                                                                                              KIND DATE
                                                                                                                                                                                                                                                     APPLICATION NO. DATE
                         PATENT NO.

EP 1170282 Al 20020109 EP 2001-114779 20010620 EP 1170282 Bl 20031001

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

DE 10032881 Al 20020117 DE 2000-10032881 20000706

AT 251121 E 20031015 AT 2001-1114779 20010626 US 2002007081 Al 20020117 US 2001-89385 20010628

JP 2002053340 A2 20020219 JP 2001-202163 20010703 CN 1341589 A 20020327 CN 2001-122837 20010706

CN 1341589 A 20020327 CN 2001-122837 20010706

DE 2000-10032881 A 20000706
R: Ar. Be. CH, De. DR. ES, FR, GB, GR, TT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO

DE 10032881 Al 20020117 DE 2000-10032881 20000706

AT 251121 E 20031015 AT 2001-1114779 20010626

US 2002007081 Al 20020117 US 2001-893858 20010628

JP 2002053540 A2 20020219 JP 2001-202163 20010703

CN 1341589 A 2 00202027 CN 2001-122837 20010706

PRICRITY APPLN. INFO:

OTHER SOURCE(S):

MARPAT 136:71544

AB 1,3,6-Hexanetricarbonitrile is prepd. by the addn. reaction of an org. adiponitrile soln. (e.g., toluene solvent) with acrylomitrile in the presence of an aq. strong base (e.g., KOH) soln. in the presence of a phase-transfer catalyst (e.g., tetrabutylammonium bisulfate).

IT 1772-25-4P, 13,6-Hexanetricarbonitrile

RI: SPN (Synthetic preparation); PREP (Preparation)

(process for the prepn. of 1,3,6-hexanetricarbonitrile)

RN 1772-25-4 CAPLUS

CN 1,3,6-Hexanetricarbonitrile (7CI, SCI, 9CI) (CA INDEX NAME)
```

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CN
NC-CH2-CH2-CH-(CH2)3-CN
```

REFERENCE COUNT:

FORMAT

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1998:598898 CAPLUS 129:289789 The kinetics and mechanism of phosphorus-catalyzed dimerization of acceptants. 1998:598658 CAPAGE 129:289789 The kinetics and mechanism of the TITLE: The kinetics and mechanism of the phosphorus-catalyzed dimerization of acrylonitrile
AUTHOR(S): Hall, C. Dennis; Lowther, Nicholas; Tweedy, Bruce R.; Hall, Adam C.; Shaw, Gordon
CORPORATE SOURCE: Dept. of Chemistry, King's College, London, WC2R 2LS, UK
SOURCE: Journal of the Chemistry (1998), (9), 2047-2054
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Iso-Pr diarylphosphinites (Ar2POPri) catalyze the dimerization of acrylonitrile (AN) to a mixt. of cis- and trans-1, 4-dicyanobut-1- ene (Cis, trans-DCB-1), trans-1, 4-dicyanobut-2-ene (DCB-2) and 2, 4-dicyanobut-1-ene (MCN). The kinetics and mechanism of the reaction, which is a potential source of hexamethylenediamine, are reported in detail and the factors which govern rate and selectivity to DCB-1 and DCB-2 rather than MGN are elaborated.

IT 68334-52-1P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; kinetics and mechanism of the phosphorus-catalyzed dimerization of acrylonitrile)
RN 68334-52-1 CAPLUS
CA -Cotene-1,3,6,8-tetracarbonitrile, 3,6-bis(2-cyanoethyl)- (7CI, 9CI) CH2-CH2-CN THERE ARE 16 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
128:218622
Use of hexanetricarboxylic acid as a complexing agent or builder in detergent formulations
INVENTOR(S):
0ftring, Alfred; Ott, Christian; Potthoff-Karl,

Birgit PATENT ASSIGNEE(S): SOURCE:

BASF A.-G., Germany Ger. Offen., 13 pp. CODEN: GWXXBX Patent German 1 DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE DE 19637428 Al 19980319 DE 1996-19637428 19960913
PRIORITY APPIN. INFO.: DE 1996-19637428 19960913
AB 1,3,6-Hexanetricarboxylic acid (I; a byproduct of acrylonitrile manuf.) or its alkali metal or ammonium salt is used as a complexing

manut.) or its alkali metal or ammonium salt is used as a complexing agent or (co)builder in laundry detergents and cleaning agents, showing improved biodegradability over EDTA. Thus, 1,3,6-tricyanohexane was hydrolyzed in 20% NaOH and acidified with concd, H2SO4 to give I. An effective cleaning agent for stainless steel brewing tanks at 60-80.degree. was prepd. by combining 50% KOH 40, 30% soln. of the tri-Ns salt of I 20, ethoxylated isotridecanol and isononanoic acid 3, aliph. carboxylic acid mixt. 3, and water 34 wt.%.

IT 1772-25-4, 1,3,6-Tricyanohexane RL: RCT (Reactant); RACT (Reactant or reagent) (use of hexanetricarboxylic acid as complexing agent or builder in detergent formulations)

RN 1772-25-4 CAPLUS
CN 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

CN | NC-CH<sub>2</sub>-CH<sub>2</sub>-CH-(CH<sub>2</sub>)<sub>3</sub>-CN

L4 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:588634 CAPLUS
129:276394
TITLE: Initiation mechanisms in free radical polymerization:
competitive reaction of cyanoisopropyl radicals with
styrene and scrylentrile

AUTHOR(S): School of Science, Griffith University, Brisbane,
4111, Australia
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry
(1998), 36(13), 2169-2176
CODEN: JPACEC; ISSN: 0887-624X
John Wiley 6 Sons, Inc.
JOURNAT TYPE: Journal
LANGUAGE: English
AB The competitive reactions of cyanoisopropyl radicals with mixed monomers
styrene and scrylentrile were studied using the nitroxide
radical trapping technique. When the trap concn. is low, second, third,
and even fourth generation (in terms of successive monomer adm), carbon
radicals were obad. as trapped products. The ratio of rate consts. for
the addn. of styrene and acrylentrile to cyanoisopropyl
radicals is 2.7 at 75.degree. and 5.3 at 105.degree. These values were
compared with the ratios for reactions of these two monomers with other
radicals and the mechanism is discussed in terms of polarity of radicals
and monomers.

IT 213918-14-4P
RL: CAT (Catalyst use): PEP (Physical, engineering or chemical process);
SPN (Synthetic preparation): PREP (Preparation): PROC (Process); USES
(Uses)
(initiation mechanism and competitive reaction of cyanoisopropyl

(Uses)
 (initiation mechanism and competitive reaction of cyanoisopropyl
 radicals with styrene and acrylonitrile in radical polymn.)
213916-14-4 CRPLUS
1,5,7-Octanetricarbonitrile, 1-{(1,3-dihydro-1,1,3,3-tetramethyl-2Hisoindol-2-yl)oxy]-7-methyl-3-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1998:90235 CAPLUS DOCUMENT NUMBER: 128:97887 Electroorganic synthesis and p. AUTHOR(S): King, Chris J. H.; Cutchens, Ci CORPORATE SOURCE: Solutia, Inc., Pensacola, FL, t Electrochemical Processing Technical Engrum. Electrolysis in the Chemical Processing Technical Engrum. Electroorganic synthesis and product recovery King, Chris J. H.; Cutchens, Charles E. Solutia, Inc., Pensacola, FL, USA Electrochemical Processing Technologies,

Forum, Electrolysis in the Chemical Industry, 11th, Clearwater Beach, Fla., Nov. 2-6, 1997 (1997), 247-258. Electrosynthesis: Lancaster, N. Y. CODEN: 650RAS

Conference

DOCUMENT TIPE: CONTESTANCE
LANGUAGE: English

AB The problems of formation unstable polymer from monomers formed from
de-cyanoethylation that leads to carbonization and fouling of column
surfaces, the instability of cyanoethylation products that leads to
refined adiponitrile (ADN) contg. unexpected level of impurities which
reduce hydrogenation catalyst activity in the electrohydrodimerization
(HMD) process are discussed. It is noted that in the cell operation it

necessary to prevent formation of reversible cyanoethylated impurities to avoid yield losses, ADN refining train fouling, catalyst poisons and undesirable impurities in refined HMD.
1772-25-49, 1,3,6-Hexanetricarbonitrile
RL: BYP (Byproduct); PEP (Physical, engineering or chemical process);

(Preparation); PROC (Process)
(electroorg, synthesis and product recovery)
1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-(CH2)3-CN

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:520920 CAPLUS
DOCUMENT NUMBER: 1293:227616
TITLE: Catalytic dimerization of acrylonitrile. I.
Homogeneous catalysts from alkyl diarylphosphinites
and dialkyl arylphosphonites
benevate of Durham, Industrial Research
Laboratories, South Road, Durham, DHI 3LE, UK
Applied Catalysis, A: General (1995), 124(2), 297-315
CODEN: ACAGE4: ISSN: 0926-860X
FUBLISHER: Elsevier
JOCUMENT TYPE: Journal
English
AB Acrylonitrile has been converted catalytically to the straight
chain dimer, 1,4-dicyanobutene-1, for the first time with both high
selectivity to the linear dimer and in high yield on acrylonitrile
consumed. The catalyst is an arom. phosphinite or phosphonite, in a
reaction medium which contains alc., hydrocarbon and acrylonitrile
and which must be purified rigorously from traces of water and phenolic
stabilizers normally present in com. acrylonitrile, otherwise
catalyst deactivation results. The catalysts were discovered during
detailed investigations into the activities of related heterogeneous
catalysts which had also been discovered to give high selectivities to
linear dimer, but in a poorly reproducible manner. The dimerization is linear dimer, but in a poorly reproducible manner. The dimerization is thought to proceed via the formation of ylide and betaine intermediates derived from the addn. of the phosphorus deriv. to acrylonitrile.

The factors affecting catalyst performance and selectivity are discussed. The product from each dimerization reaction was a mixt. his- and trans-1,4-dicyano-1-butene, 1,4-dicyano-2-butene, 1,3-dicyano-1-butene, hexa-acrylenitrile, and others.
68334-52-1P
RL: BYP (Byproduct): PREP (Preparation)
(catalytic dimerization of acrylenitrile using alkyl
diarylphosphinite and dialkyl arylphosphonite catalysts)
68334-52-1 CAPLUS
4-Octene-1,3,6,8-tetracarbonitrile, 3,6-bis(2-cyanoethyl)- (7CI, 9CI) INDEX NAME) . с-сн=сн-NC-CH2-CH2-C- CH2- CH2- CN NC-CH2-CH2 CH2-CH2-CN

AUTHOR(S): Jitaru, Maria; Ciomos, Florentina; Oprea, Ovidiu Horea; Toma, Bogdan C.; Toma, Mariana Dep. Phys. Chem., Univ. Cluj-Napoca, Cluj-Napoca, CORPORATE SOURCE: SOURCE: Bep. Phys. Chem., with City-Rapoca, Ety-Rapoca, Rom.

Revue Roumaine de Chimie (1990), 35(7-9), 859-66

CODEN: RRCHAX; ISSN: 0035-3930

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Comparative expts. of acrylentrile electroredn. on Pb vs. PbO2

electrodes in neutral phosphate buffer, with - or without cationic surfactants demonstrated that the selectivity of the process is essentially under the control of the quality and quantity of the quaternary ammonium salt added. Thus, in the absence of surfactants, the process is directed towards the non-dimerizant electroredn. leading with high selectivity to propionitrile, whereas at levels of about ten times the crit. micellar concm. the surfactant ensures a preponderant formation of the electrohydrodimerization products: adiponitrile and traces of methylglutaronitrile. At the same time, the phase transfer catalysis effect exerted by the surfactant entails, besides a favorable influence Rom. SOURCE: DOCUMENT TYPE: the dimerizant electroredn., an increased formation of water condensity action products.

1772-25-4P, 1, 3, 6-Tricyanohexane
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, as impurity, in electrochem. redn. of
acrylonitrile in presence of alkyltrimethylammonium surfactant)
172-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME) NC-CH2-CH2-CH-(CH2)3-CN

L4 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:417462 CAPLUS
DOCUMENT NUMBER: 115:17462
TITLE: Effect of surfactants on the electroreduction of acrylonictrile oniciu, Liviu; Silberg, Ioan A.; Lowy, Dan A.;

L4 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:57109 CAPLUS
DOCUMENT NUMBER: 110:57109
TITLE: 10:57109
Preparation of 4-aminomethyl-1,8-diaminooctane
Yamataka, Kazunori; Oshima, Shozo
Asahi Chemical Industry Co., Ltd., Japan
Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: 7AMILY ACC. NUM. COUNT: 1 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: KIND DATE APPLICATION NO. JP 62270550 A2 19871124 JP 1986-113592 19860520 JP 07045440 B4 19950517 PRIORITY APPLM. INFO.: JP 1986-113592 19860520 OTHER SOURCE(S): CASREACT 110:57109

AB H2N(CH2)3CH(CH2NH2) (CH2)4NH2 (I), useful as an epoxy curing agent, anticorrosive agent, etc. (no data), was prepd. by electrolytic redn. of CH2:CHCN (II) in the presence of quaternary ammonium salts, elimination of NC(CH2)4CN (III) to .ltoreq.2% from the electrolytic soln. contg. III and NCCH2CH2CH(CN)CH2CH2CH2CN (IV), mol. distn. of IV from the high b.p. residue, and liq. phase hydrogenation of IV in the presence of Raney catalysts. Thus, electrolysis was carried out in an electrolyzer contg. 101 aq. H2SO4 anolyte and a catholyte which consisted of a 2:8 (by vol.) org. phase/aq. phase emulsion [org. phase omposed of II, III, EtCN, IV, and H2O; aq. phase contg. (Et4N)2SO4). After electrolysis for 2000 h, and IV were produced in 89% and 7.0% yield, resp. Then, III was removed from the electrolytic soln. by distn. in 82% removal ratio to give a high b.p. residue contg. 1.38% III, which was applied to mol. distn. to give a distillate contg. 96.0% IV. Then, the distillate was autoclaved in the presence of Raney Co and H2O under H at 150.degree. for 180 min to give 69% II (based on IV). 1772-25-49, 1,3,6-Hexanetricarbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (Reactant or reagent) sew (synthetic preparation); PREP (Preparati (Reactant or reagent) (prepn. and hydrogenation of, in presence of Raney catalysts) 1772-25-4 CAPLUS 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

109:192566
Selective process for epoxidation of styrene to styrene oxide
Barbe, Claude Edouard: Golitsch, Maria de Lourdes;
Alkawa, Lumi Tsuchiya
Rhodia S. A., Brazil
Braz. Pedido PI, 10 pp.
CODEN: BPXXDX
Patent INVENTOR (S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent Portuguese 1 PATENT NO. KIND DATE APPLICATION NO. DATE

BR 8500801 A 19860923 BR 1985-801 19850215

PRIORITY APPLN. INFO.: BR 1985-801 19850215

AB Styrene oxide is prepd. in high yields by the epoxidn. of styrene with H202 in the presence of a nitrile (0.3-1.35 mol/mol styrene) in an elc. medium maintained at pH 8.8-10.0 by adding an aq. alkali metal hydroxide soln. Suitable nitriles are the 1,3,6-tricyanchexane-contg. byproduct of the manuf. of adiponitrile and byproducts of the manuf. of adiponitrile.

IT 1772-25-4

RI: USES (Uses)

(in styrene oxide manuf. from styrene) (in styrene oxide manuf. from styrene)
1772-25-4 CAPUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1988:592566 CAPLUS
DOCUMENT NUMBER: 109:192566
TITLE: Selective process for epoxidat.

NC-CH2-CH2-CH- (CH2) 3-CN

NC-CH2-CH2-CH-(CH2)3-CN

SOURCE:

L4 ANSWER 17 OF 39
ACCESSION NUMBER:
D96:1806673
ACIDEN
AUTHOR(S):
AUTHOR(S):
COPPORATE SOURCE:
USA

SOURCE:
CAPLUS COPYRIGHT 2003 ACS on STN
1982:180673 CAPLUS
96:180673 CAPLUS
96:180673 CAPLUS
1982:180673 CAPLUS
1982:180

USA Journal of the American Chemical Society (1982), 104(9), 2675-6 CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE:

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title process involved the sequence NCCH2- + CH2:CHCN .fwdarw. m/z 93
.fwdarw. m/z 146 .fwdarw. m/z 199 .fwdarw. m/z 252. Termination of the
telomerization occurred at the tetrameric anion, and apparently resulted
from intramol. ion-dipole assocn. of the anion growing end, -CHCN-, with

cyano groups on the telomer backbone. The data were simulated by computer, yielding the rate consts. for each step and an upper limit for the further telomerization of the tetrameric anion. 81388-06-99

IT

RI: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
1388-06-9 CAPLUS
1,3,5,7,9-Nonanepentacarbonitrile, ion(1-) (9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-CH2-CH-CH2-CH-CH2-CH-CH2-CH

L4 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:184858 CAPLUS

106:184858 CAPLUS

106:184858 CAPLUS

106:184858 CAPLUS

Selectivity characteristics of the electrohydrodimerization of acrylonitrile

Scott, K.; McConvey, I. F.; Henderson, J.

DOP. Chem. Eng., Teesside Polytech, Middlesbrough/Cleveland, TSI 3BA, UK

329-39

CODEN: JAELBJ; ISSN: 0021-891X

JOURNET TYPE:

CODEN: JAELBJ; ISSN: 0021-891X

DOCUMENT TYPE: Journal
LANGUAGE: English
AB A math. model of a reaction scheme for the electrohydrodimerization of
acrylonitrile to adiponitrile in a loop reactor is presented.

This model, which is based on a plug flow reactor with a recycle loop and
continuous removal of the product, is used to simulate steady-state
operation at various operating conditions. The effect of flow rate, c.d.
and mass transport were investigated in terms of their effect on product
distributions and selectivity. Overall, the reaction model deals with

formation of 5 products from the cathodic reactions.
1772-25-4, 1,3,6-Tricyanohexane
RL: PROC (Process)
(transformation of, in electrohydrodimerization of
acrylonitrile, math. model for)
1772-25-4 CAPLUS
1,3,6-Hexanetric

NC-CH2-CH2-CH-(CH2)3-CN

L4 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1981:514820 CAPLUS
DOCUMENT NUMBER: 95:114820
Adiponitrile from 1,3,6-tricyanohexane
Asahi Chemical Industry Co., Ltd., Japan
Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

Japanese 1

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE JP 56040656 A2 19810416 JP 1979-116687 19790913 JP 62015068 B4 19870406 JP 1979-116687 19790913 Adiponitrile (I) was recovered from pyrolysis of 1,3,6-tricyanohexane (II)

at 300-420.degree. in the liq. phase or at 400-600.degree. in the gas phase with or without a catalyst. Thus, silica gel contg. 1.5% NaOH was pelletized with bentonite, packed into a glass tube, and treated with 2 g II/h-mL catalyst at 450.degree./20-40 mm to give 53.6% I and 49.9% accylonitrile with 81.9% conversion. K2CO3, MgO, KOH, KCN, Pt, V2O5, or C12O3 was also used.

1772-25-4
RL: RCT (Reactant): RACT (Reactant or reagent)
(pyrolysis of, adiponitrile from)
1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI. 8CI. 9CI) (CA INDEX NAME)

1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-(CH2)3-CN

L4 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN ACCESSION NUMBER: 1979:465194 CAPLUS DOCUMENT NUMBER: 91:65194 The Phillip's process for the electrohydrodimerization

THE PAILIE's process for the electrohydrodimerization of acrylonitrile

AUTHOR(S): Childs, W. V.: Walters, H. C.
CORPORATE SOURCE: Phillips Pet. Co., Bartleaville, OK, 74004, USA
SOURCE: ATCHE Symposium Series (1979), 75(185), 19-25

CODEN: ACSSCQ: ISSN: 0065-8812

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The Phillips' electrochem. process for converting acrylonitrile to adiponitrile employs an undivided cell with Pb electrodes and offers lower investment and lower energy costs compared to other similar processes. The electrolysis cell used in the process is described. The electrolyte is K phosphate with a trace of Bu4N+. The yield of adiponitrile depended on acrylonitrile level pH, tetraalkylammonium concn. and compn., electrolyte concn., c.d., and linear

tetraalkylammonium concn. and comput, exector, execution the call. The optimized efficiency was >90% which is comparable to other electrohydrodimerization processes. The terminal voltage was 4.0 V at 2 kA/m2 and 50.degree.

IT 172-25-4P
RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in aerylonitrile electrohydrodimerization)
RN 1772-25-4 CAPLUS
CN 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

CN | | CH2-CH2-CH-(CH2)3-CN

ACCESSION NUMBER: 1978:23446 CAPLUS
DOCUMENT NUMBER: 88:23446 SAPLUS

BALTATED ACCESSION NUMBER: 1978:23446 CAPLUS
DOCUMENT NUMBER: 88:23446

AUTHOR(S): Saturated oligomers

AUTHOR(S): Balard, Henri: Meybeck, Jean

CORPORATE SOURCE: Lab. Chim. Org. Ind., CNRS, Mulhouse, Fr.

SOURCE: EULOPAGE POLYMER JOURNAL (1977), 13(7), 617-21

CODEN: EURJAG; ISSN: 0014-3057

DOCUMENT TYPE: JOURNAL

LANGUAGE: French

AB Eleven compds. RCH(CN)(CR2CH(CN))RRI (I) were prepd. from the unsatd.

CH2:CHCN oligomers. The unsymmetric compds. I (R = Me, Rl = H; n = 1-3),

e.g. MeCH(CN) [CH2CH(CN)] 3H [64018-23-6] were prepd by

hydrogenation of CH2:C(CN)[CH2CH(CN)]nR and condensation of 1 or 2 mols.

unsatd. oligomer with tert-Bu cyanoacetate (1116-98-9) followed by

pycyclysis gave I (R = Rl = Me) R = R = H: N n = 1-4), e.g.

MeCH(CN)[CH2CH(CN)]2Me [17199-93-8] and CH2(CN)[CH2CH(CN)]2H

[4379-34-8].

IT 48918-28-99 64918-28-1P 64918-30-5P

64936-51-2P

64918-26-9P 64918-28-1P 64918-30-5P 64936-31-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and pyrolysis of) 64918-26-9 CAPLUS Octanoic acid, 2,4,6,8-tetracyano-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

O CN CN CN || | | | | -C-CH-CH2-CH-CH2-CH-CH2-CH2-CN

64918-28-1 CAPLUS

Heptanoic acid, 2,4,6-tricyano-2-(2,4-dicyanopentyl)-, 1,1-dimethylethylester (9CI) (CA INDEX NAME)

64918-30-5 CAPLUS Hexanolc acid, 2,4,6-tricyano-2-(2,4-dicyanobutyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1979:88043 CAPLUS
DOCUMENT NUMBER: 90:88043 Thermal conversion of 4-cyano-suberonitrile to acryl-onitrile

INVENTOR(S): Campbell, Charles R.; Heckle, William A.; Mathews, Marion J.

PATENT ASSIGNEE(S): Monsanto Co., USA
SOURCE: U.S., 4 pp..
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

105 4128571 A 19781205 US 1977-946100 19771027

PRIORITY APPLN. INFO: US 1977-946100 19771027

AB 4-Cyanosuberonitrile (I) [1071-25-4] is continuously converted to accylentifie (II) [107-13-1] in a catalyst-free reaction at 700-800.degree. and vol. hourly space velocity (YHSV) 2600-8000. Thus, a mixt of I 70.5, adiponitrile 2.5, and other materials 27% was fed into a 10 ft .times. 0.25 in. stainless steel tube at 750.degree. and VHSV 2632 (contact time 1.37 s) to give 30.9% II. Optionally, the feed mixt can contain .ltoreq.2 parts propionitrile [107-12-0] diluent per part of the above feed mixt.

IT 1772-25-4

RI: PROC (Process)
(Chermal conversion of, to acrylenitrile, noncatalytic)

RN 1772-25-4 CAPLUS

CN 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

CN | |NC-CH<sub>2</sub>-CH<sub>2</sub>-CH-(CH<sub>2</sub>)<sub>3</sub>-CN

L4 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

64936-51-2 CAPLUS Nonanoic acid, 2,4,6,8-tetracyano-2-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

64000-86-8P 64000-87-9P 64918-23-6P 64918-24-7P 64918-25-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
64000-86-8 CAPLUS
2,4,6,8-Nonanetetracarbonitrile (7CI, 9CI) (CA INDEX NAME)

64000-87-9 CAPLUS 2,4,6,8,10-Undecanepentacarbonitrile (9CI) (CA INDEX NAME)

64918-23-6 CAPLUS
1,3,5,7-Octanetetracarbonitrile (9CI) (CA INDEX NAME)

CN CN CN CH-CH2-CH2-CN CN

64918-24-7 CAPLUS
1,3,5,7-Heptanetetracarbonitrile (6CI, 9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

NC- CH2- CH2- CH- CH2- CH- CH2- CH2- CN

64918-25-8 CAPLUS 1,3,5,7,9-Nonanepentacarbonitrile (9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
1978:7439 CAPLUS
Synthesis of polyacrylonitrile oligomers. I.
Unsaturated oligomers
CORPORATE SOURCE:
SOURCE:
CORPORATE SOURCE:
Lab. Chim. Org. Ind., CNRS, Mulhouse, Fr.
European Polymer Journal (1977), 13(7), 611-15
CODEN: EUPJAG; ISSN: 0014-3057
JOURNAL
AB Five oligomers CH2:CCN(CH2CHCN)nR (R = H or Me, n = 1-3), e.g.
2,4-dicyano-1-pentene [35299-21-9], were prepd. by Bu3P catalyzed anionic oligomerization of ecrylenitrile (107-13-1] and by Feit's iterative method. The 2 synthesis methods were discussed and the products

products
were characterized by chromatog, and IR and NMR spectroscopy.

IT 6918-32-7P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) 64918-32-7 CAPLUS 7-Octene-1,3,5,7-tetracarbonitrile (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:518331 CAPLUS
DOCUMENT NUMBER: 87:118331

AUTHOR(S): Determination of the tacticity of polyacrylonitrile and its oligomers by carbon-13 NNR spectroscopy

AUTHOR(S): Balard, Henri; Fritz, Hans; Meybeck, Jean

CORPORATE SOURCE: Lab. Chim. org. Ind., Ec. Super. Chim., Mulhouse, Fr.

SOURCE: CODEN: MACEAK; ISSN: 0025-116X

DOCUMENT TYPE: Journal

LANGUAGE: Briglish

AB The microtacticity of polyacrylonitrile (I) [25014-41-9] and its model: compds., the dimer [15074-49-4], trimer [17199-93-8], and tetramer [
64000-65-8] of acrylonitrile were detcd. by 13C NNR

spectroscopy. In the case of the oligomers, the carbons of the chain are the most stereosensitive ones, but for I the carbon of the cyano group

the most stereosensitive. The 13C NMR spectrum of I was composed of 10 peaks which can be assigned to the 10 possible pentad configurations.

64000-86-8
RL: PRP (Properties)
 (tacticity of, detn. of, by carbon-13 NMR)
64000-86-8 CAPLUS
Z,4,6,8-Nonanetetracarbonitrile (7CI, 9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1976:45883 CAPLUS
ACCESSION NUMBER: 43:45883
ACTYLIC fibers
SINVENTOR(S): 5himizu, Kunitoshi; Iwasa, Toshio; Seki, Shuji
ASAİn Chemical Industry Co., Ltd., Japan
JDCLUMENT TYPE: COPEN: JKXKAF
DOCUMENT TYPE: Patent INFORMATION: 1
FAMILU ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 50111148 A2 19750901 JP 1974-13621 19740204

PRIORITY APPLN. INFO.: JP 1974-13621 19740204

AB Melt spinning blends contg. an acrylic polymer [contg. mainly acrylonitrile [1] units] and a I trimer, e.g., 1,3,6-tricyanohexane (II) [1772-25-4], or mixts. of oligomeric polyacrylonitrile [25014-41-9] contg. the trimer gave fibers with increased tensile attength. Thus, a mixt. contg. I 95, Me acrylate (III) 5, II 80, and tetr-Bu percoxypivalate 1.5 parts was polymd, 10 hr at 70.degree. to give a polymer (IV) [24968-79-4] mixt. IV mixt. (contg. 43)

II) was spun at 169.degree. and the spun fibers were drawn 200% in H2O at 100.degree. and heated 1 min at 135.degree. to give 2.7-denier/filament fibers with tenacity 4.81 g/denier and elongation 13.5%. Yinyl acetate-1 copolymer [24980-62-9], Me methacrylate-I copolymer [30396-85-1], Na allyisulfonate-I-III copolymer [25035-78-5], 2-vinylpyridine-I copolymer [2636-60-2], and vinylidene chloride-I copolymer [9010-76-8] were also

[20830-00-2], and analyze used.
1772-25-4
RE: USES (Uses)
(blends with scrylic polymers, spinning of, for increased tensile strength)
1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-(CH2)3-CN

L4 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1969:480616 CAPLUS
TITLE: Electrolytic reductive oligomerization of serylonitrile and related olefins
Baizer, Manuel M.
CORPORATE SOURCE: Cent. Res. Dep., Monsanto Co., St. Louis, Mo, USA World Petrol. Congr., Proc., 7th (1968), Meeting Date 1967, Volume 5, 311-16. Elsevier Publ. Co. Ltd.:
Barking, Engl.
CODEN: 21GMA6
CODEN: 21GMA6
CODEN: 21GMA6
CODEN: 21GMA6
CODEN: 21GMA6
CODEN: 21GMA6
DOCUMENT TYPE: Conference
English
AB The electrolytic reductive oligomerization of concd. solns. of acrylonitrile in hydrotropic electrolytes has been studied over a range of H2O concns. At high H2O content, propionitrile is the main redn.
product; at intermediate concns., almost quant. yields of adiponitrile are obtained; in nearly anhyd. media hydrotrimer, hydrotetramer as well as low-melting acrylonitrile polymers are formed. The probable mode of formation of this range of products is discussed. Electrolytic reductive dimerization was extended to include all monomeric activated olefins in which the activating group is itself not reduced; higher oligomerization was sought for and demonstrated in only a limited number of cases. The acrylonitrile dimer, alpha.—methyleneglutaronitrile, underwent electrolytic reductive dimerization to yield an acrylonitrile to yield argylonitrile by hydroterimer. The formation of oligomers from acrylonitrile on treatment with catalytic quantities of tertiary phosphines is discussed. The relevant literature on non-electrolytic methods for oligomerizing activated olefins is cited.

IT 1572-42-55 1572-43-65 1772-25-48
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 1572-43-6 CAPLUS
CN 1,3,5,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1972:85349 CAPLUS
DOCUMENT NUMBER: 76:85349

TITLE: Identification of high-boiling impurity in adipodinitrile, obtained from accylonitrile
AUTHOR(5): Usowa, E. P.; Upadysheva, A. V.; Mitina, L. I.;
Grigor'eva, N. D.; Znamenskaya, A. P.

CORPORATE SOURCE: USSR
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1971), 44(11), 2598-9

CODEN: ZPKHAB; ISSN: 0044-4618

DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB 1,3,6-Tricyanohexane (I) was sepd. from adipodinitrile by preparative liq.
chromatog. on Al203. I was also obtained by heating 1-amino-2-cyano-1-cyclopentene and acrylonitrile in C6H6 with a catalytic amt. Na 6-8 hr at 80.degree.

IT 1772-25-4 CAPLUS
CN 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CN

NC-CH2-CH2-CH2-CH (CH2)3-CN

L4 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1969:439500 CAPLUS
DOCUMENT NUMBER: 71:39500
TITLE: Telomerization of acrylonitrile by
N.N-dichloro-p-chlorobenzenesulfonamide
AUTHOR(S): Rybakova, N. A.: Freidlina, R. Kh.
CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR
SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR
(1969), (5), 1194-5
CODEN: IASKA6: ISSN: 0002-3353
DOCUMENT TYPE: CODEN: IASKA6: ISSN: 0002-3353
DOLINAL
AB Heating 13 g. -CLG6H4SO2NC12 with 5.3 g. CH2:CHCN and 1.43 g.
dicyclohexyl peroxydicarbonate in CC14 under N at 60-5.degree. for 1.5
hrs. gave a solid, which after washing with more CC14 gave after
with EtOH 1.9 g. sol. C24H23C12N702s, m. 135-40.degree., and alc.-insol.
material that was not identified. The sol. fractions were fractionated
from CC14 to yield 2.8 g. p-C166H4SO2NHCH2CHCICN and 2.5 g.
p-C1C6H4SO2NHC(2CH(CN))2Cl, m. 68.degree., and mixed analogous telomers
with 3-5 links of the acrylonitrile component, which were not
sepd. From other similar runs with varying proportions of starting
materials were isolated similar telomers from n = 1 to n =>6. The
following were isolated in the pure state: p-C1C6H4SO2NH(CN)InCl: n
= 7, decompd. 205-15.degree.; n = 9, decompd. 190-200.degree.; n = 14,
decompd. 205-15.degree. Ir spectra are reported.

IT 24729-16-6 24729-17-79 24729-18-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 24729-16-6 CAPLUS
CN Benzenesulfonamide,
p-chloro-N-(12-chloro-2,4,6,8,10,12-hexacyanododecyl)(8CI) (CA INDEX NAME)

PAGE 1-B

24729-17-7 CAPLUS Benzenesulfonamide, p-chloro-N-(14-chloro-2,4,6,8,10,12,14-heptacyanotetradecyl)- (8CI) (CA INDEX NAME)

L4 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1968:96360 CAPLUS
DOCUMENT NUMBER: 68:96360 CAPLUS
TITLE: Polyacrylonitrile
BAIZET, Manuel M.
Monsanto Co.
U.S., 6 pp.
COODEN: USXXAM
PACHOLING PACHOLING:
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE

(prepn. of) 1772-25-4 CAPLUS 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-- CH2-- CH2-- CH-- (CH2) 3-- CN

ANSWER 28 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-R

24729-18-8 CAPLUS Benzenesulfonamide, p-chloro-N-(18-chloro-2,4,6,8,10,12,14,16,18-nonacyanoctadecyl)- (8CI) (CA INDEX NAME)

PAGE 1-B

L4 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
1967:76086 CAPLUS
CORPORATE
AUTHOR(S):
CORPORATE SOURCE:
Shell Grundlagenforsch. Ges., Schloss Birlinghoven,
Siegburg, Germany
Tetrahedron Letters (1966), (51), 6347-51
CODEN: TELEAT; ISSN: 0040-4039
DOCUMENT TYPE:
JOURNAL
LANGUAGE:
AUX Mixts. of H2C:CHCN and various diaryl and arylalkyl phosphinites, RRIPOR2
(I) in Me3COH contg. 50 mg. hydroquinone stirred (N atm.) became intensely yellow and after a short induction period reacted exothermically to reflux

themp. with sepn. of a cryst. hexamer (II) and oily polymers. After cessation of the exothermic reaction in 1-2 hrs. the mixt. was filtered and the filtrate distd. to yield unreacted H2C:CHCN, a crude fraction of

and the filtrate distd. to yield unreacted Recience, a group fraction of 2

acrylonitrile dimers and phosphinite secondary products. Extn. with MeCN sepd. II from the polymers. The % yields of II, dimers, and polymers were tabulated. Whereas in the absence of solvent extremely vigorous polymn, to a brown resin occurred, in the presence of Me3COH the reaction gave 6.2-41.3% yields of II, i.e.,

1,4,4-tetrakis(2-cyanocthy1)1,4-dicyano-trans-2-butene, m. 241-3.degree. (HCCNNe2-MeCN). I (R = R1 = p-MeC6H4, R2 = Et) and I (R = R1 = Ph, R2 = Et) gave the 28% yields with small amts. of polymer, whereas I (R = R1 = Ph, R2 = CH2CMe3) and I (R = Ar, R = alk., R = Et) gave much polymer with practically complete conversion of H2C:CHCN. All diarylphosphinites independent of the ester groups in the presence of Me3COH gave a quant. yield of Ar2D(0)CH2CH2CH: Ar = Ph, m. 102-3.degree. (C6H6), b0.02 215-19.degree., M+ 255, and Ar = p-MeC6H4, b0.5 240.degree. M+ 283. Ph2PSEt and Ph2POP gave no oligomerization with H2C:CHCN. The reaction of Ar2POR with CH2:CHCN took place in accordance with the mechanism proposed by Takashina and Price (CA

56, 14075b). 15590-02-0P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
15590-02-0 CAPLUS
4-Octene-1,3,6,8-tetracarbonitrile, 3,6-bis(2-cyanoethyl)-, (E)- (8CI)
(CA INDEX NAME)

Double bond geometry as shown.

ORIGINAL ACC. NUM. COUNT:
PATENT ACC. NUM. COUNT:
PATENT INFORMATION:

PATENT INFORMATION:

PATENT NO. KIND DATE

US 3245889

Polymers of low mol. wt. are prepd. by controlled electrolysis of catholytes which are coned. solns. contg. accylonitrile (I), and electrolyte salt, and a compd. that provides a relatively low concn. of protons. The process is generally carried out in the absence of free-radical-generating catalysts and of anions (except carbanions formed in the reaction) capable of catalyzing anionic polymerization of I. Inhibitors of free-radical catalysis may be present. Polymerization proceeds as a result of addn. of 2 electrons to a mol. of I to form a dicarbanion, which then reacts with addnl. I to give a cross-linked configuration. Termination of the polymerization process may be accomplished by increasing the concn. of protons, which add to the carbanion chains and inhibit further reaction. Aryl- and alkarenesulfonic acid salts are esp. suitable for use in anolyte solns., which are sepd. from the cathodic half-cell by a semipermeable membrane or divider. For example, in a jacketed glass vessel contg. 110 ml. Hg as the cathode, a catholyte was placed consisting of a soln. of I (contg. a trace of p-nitrosodimethylaniline) 23.1, tetraethylammonium p-toluenesulfonate

(II) Strong August 2015 and 120 feet to be butter and the toward at the cathod and the confidency of the content of the confidency of the controlled of the cathodic half-confidency of the confidency of the

25, HCONMe2 (III) 82.3, and H2O 2.6 g. An Alundum cup immersed in the catholyte contained 15 ml. of 80 wt. % II dild. with 5 ml. H2O as the anolyte. A Pt anode was immersed in the anolyte. The anode and cathode were connected, resp., to the pos. and neg. terminals of a d.c. source.

current of 0.1-0.5 amp. at a cathode voltage of -1.5 to -1.6 (vs. a satd. Hg2Cl2 electrode) was passed through the cell for a few min. with no apparent reaction. The voltage was then increased to cause a 1.4-amp. current to flow (at -1.85 v.), and the catholyte temp. rose to >40.degree. Electrolysis was discontinued after 1.45 amp.-hrs. and the catholyte was dild. with 300 ml. cold H2O. The resulting polymer was collected by filtration, washed with H2O, and dried to a wt of 13.1 g. The product (m. 115-40.degree. osmometric mol. wt. 714) contained C 3.

4. H 6.20, and N 25.15%, indicating a mol. of .apprx.14 units of I with the formula H(C3H3N)14H. It was sol. in Me2CO, acetonitrile (IV), concd.

and Ac20. When the procedure of the above example was repeated with IV instead of III as cosolvent, the polymer formed did not sep. from the abath, indicating that IV and H20, together in the catholyte, furnished sufficient protons to terminate polymerization at a very early stage.

L4 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1966:104097 CAPLUS
DOCUMENT NUMBER: 64:104097
CORIGINAL REFERENCE NO: 64:19568h, 19569a
NICOLINIC ACID NICOLINIC ACI

KIND DATE APPLICATION NO. DATE US 3246000 19660412 US 19631218
A process is described for the prepn. of nicotinic acid (I) from acrylonitrile (II). Thus, electrolysis of a catholyte of 60 g. tetracetylammonium probluenesulfonate, 3 g. H2O, and 160 g. II and an anolyte of 30 ml. 82% methyltributylammonium methylsulfate in 20 ml. H2O with 1.5-2.0 amp. for 3.5 amp.-hrs., the mixt. dild. with H2O, extd. with CH2C12, and the ext. fractionated to give as one fraction 1,3,6-tricyanohexane (III), bO.2 186-200.degree. III was heated 24 hrs. at 150.degree. and 3000 psi. with Raney Co and H, the mixt. distd. to

1,8-diamino-4-aminomethyloctane (IV), b0.2-0.25 98.5-103.0.degree., n27D 1.4822 and a small amt. of 3-(4-aminobutyl)piperidine (V), di-HCl salt m. 228.8-30.0.degree.. Hydrogenation of IV in the presence of NH3 gave V. Acetylation of V with Ac20 followed by dehydrogenation with H01 Pd on C

200.degree. gave 3-(4-acetylaminobutyl)pyridine (VI). Oxidn. of VI with

IT

HNO3 gave I. 1772-25-4, 1,3,6-Hexanetricarbonitrile (prepn. of) 173-25-4 CAPLUS 173,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-(CH2)3-CN

ANSWER 31 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Polymers suitable for low-temp. molding and coating operations can be prepd. in this way.

1572-42-5, 1,3,5,8-Octanetetracarbonitrile 1572-43-6,
1,3,6,8-Octanetetracarbonitrile 1772-25-4, 1,3,6Hexanetricarbonitrile
(formation in acrylonitrile soln. electrolysis)
1572-42-5 CAPLUS
1,3,5,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

NC-CH2-CH2-CH-CH2-CH-(CH2)3-CN

1572-43-6 CAPLUS
1,3,6,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

-сн-сн<sub>2</sub>-сн<sub>2</sub>-сн-сн<sub>2</sub>-сн<sub>2</sub>-сп

1772-25-4 CAPLUS 1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

CN | NC-CH<sub>2</sub>-CH<sub>2</sub>-CH-(CH<sub>2</sub>)<sub>3</sub>-CN

L4 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1965:409761 CAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.:

63:9761 63:1695e-h,1696a-c

Syntheses with trichloroacetonitrile Coenen, Nax: Faust, Juergen; Ringel, Christian; AUTHOR (S):

Mayer,

CORPORATE SOURCE: SOURCE:

roland Tech. Univ., Dresden, Germany Journal fuer Praktische Chemie (Leipzig) (1965), 20715-6), 239-50 CODEN: JPCEAG: ISSN: 0021-8383 Journal

DOCUMENT TYPE:

MENT TYPE: Journal UAGE: German German A series of compds. of the general type CCl3C(NH2):CRR' (I) was prepd. by the addn. of the appropriate CH-acidic compds. to CCl3CN (II) whereby an Ac group can be cleaved off acetolytically. Certain amines eliminate the CCl3 group in I as CHCl3 and lead to the corresponding R' NHC(NH2):CRR' (III). Several 2-substituted 3-amino-3-hydrazinoacrylic acid esters and nitriles were cyclized to pyrazoles. II (50 g.) and 30 g. CH2(CN)2 in

cc. MeOH treated with stirring with 100 cc. H2O and 5 cc. satd. aq. AcONa and the mixt. stirred about 5 min. gave 54 g. I (R = R' = CN), m. 196.degree. [aq. HCONMe2 (DMF) or iso-PrOH]. Similarly were prepd. trans-I (R = CN, R' = COZMe) (IV), 804, m. 145-6.degree. (iso-PrOH), and cis-I (R = BZ, R' = CN), 754, m. 180.degree. (aq. iso-PrOH). BECHZCOZEt (14 g.) and 10.5 g. II in 60 cc. MeOH stirred 0.5 hr. with 20 cc. satd. aq. AcONa and the mixt. heated 5 min. at 60.degree. gave 12 g. trans-I (R = CO2EL, R' = BZ) (V), m. 100-1.degree. (EtOH). Ac2CH2 (50 g.) and 70 g. II in 200 cc. MeOH strated with stirring with 100 cc. satd. aq. AcONa during 2 hrs. gave 78 g. CCl3C(NH2):CHR (VI) (R = Ac). AcCH2CO2Me with

gave similarly 55% VI (R = CO2Me), m. 53-4.degree. (aq. iso-PrOH). AcCH2Bz and II (equimolar amts.) yielded 60% VI (R = Bz), m.

102 (aq. iso-PrOH). The appropriate I (0.1 mole) added with stirring to 0.25 mole suitable amine and the mixt. heated 5 min. on the water bath gave

corresponding III (R = CO2Me, R' = CN) (R'', m.p., and % yield given):

131.degree. (1:1 aq. DMF), 65; iso-Pr, 106.degree. (3:1 MeOH-H2O and 1:1 iso-PrOH-H2O), 80; iso-Bu, 123.degree. (MeOH), 95; CH2:CHCN2, 110.5.degree. (MeOH), 80; Am, 146.5.degree. (MeOH), 90. Similarly was prepd. III (R = Bz, R' = CN, R'" = PhCH2), m. 199-200.degree. (MeOH), 95. The appropriate I (0.1 mole) in DMF treated with stirring with a suitable amine or with N2H4.H2O and the mixt. dild. after 10 min. with H2O gave

corresponding III (R, R', R', m.p., % yield, cc. DMF, g. am N2H4.H2O, and cc. H2O used are given): C02Me, CN, NH2 (VII),

N2H4.H2O, and cc. H2O used are given): CO2Me, CN, NHZ (VII),
171-3.degree. (MeOH), 70, 185, 10, 670; Bz, CN, NH2, 157-61.degree. (H2O), 70, 145, 15,
430; CO2Et, Bz, CHZCHZOH, 136-7.degree. (C6H6), 85, 170, 31, 675; CO2Et,
CO2Et, NH2, 114-15.degree. (H2O), 65, 245, 15, 380. IV (0.1 mole) in 130
cc. DMF treated dropwise with stirring with 5 g. MeNHZ in 100 cc. DMF and
the mixt. after 10 min. heated at 70-5.degree. for 3 min. gave 14.1 g.
trans-III (R = CO2Me, R' = CN, R' = Me), m. 155-6.degree. (H2O). IV
(85.2 g.) added with stirring and cooling to 50 g. EtNHZ and the mixt.
heated 0.5 hr. on the water bath gave 42.5 g. trans-III (R = CO2Me, R' =
CN, R'' = Et) (VIII), m. 132.5-33.degree. (30% ag. MeOH). (CH2NHZ)2 (12
g.) treated with stirring with 84 g. IV (after 42 g. had been added, the

ANSWER 33 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) mixt. was dild. with 30 cc. CRCl3) and heated 5 min. on the water bath yielded 4.7 g. yellow [Meo2C(NC)C:C(NH2)NNCR2]2, m. 284-8.degree. (decompn.) I (R = R\* = COZEL)2 (2 g.) added to 4 g. H2NCHZACHOM and the mixt. heated with stirring to soln., cooled, and dild. with 10 cc. H2O in portions gave 1.3 g. III (R = R\* = COZEL; R\*\* = CHZCHZOH), m. 107-8.degree. (C6H6). IV (20 g.) in 100 cc. 101 aq. NaOH kept 3 days at room temp gave 2.2 g. CRCl3; the aq. phase neutralized with concd. HCl gave 2 g. unreacted IV; further acidification to pH 2 gave 3 g. brownish H2NC(OH):C(CN)COZMe, m. 110-12.degree. (xylene). VIII (11.8 g.), 85 cc. concd. H2SO4, and 150 cc. H2O treated with stirring during 0.5 min. at 10-15.degree. with 4.85 g. NaNO2 in 15 cc. H2O yieled 4.85 g.
ELNNC(OH):C(CN)COZMe, m. 11-21.3-28.5-degree. (ligroine, b. 80-90.degree., and then H2O). VII (15.6 g.) added as rapidly as possible to 300 cc. refluxing PhOEt and the mixt. refluxed 140 min. yielded 15.45 g.
3,5-diamino-4-carbomethoxypyrarole (1x), m. 231-2.degree. IX stirred

hr. with excess BzCl in C5H5N gave 40% 3-BzNH analog of IX, m.

183-6.degree. (MeOH). V (2 g.) in 8 cc. DMF treated with 1 cc. N2H4.H2O and then shaken with 30 cc. H2O yielded 1.2 g. 3-amino-4-carbethoxy-5-phenylpyrazole (X), m. 167-9-degree. (C6H6). X (2 g.) in 25 cc. 4N NaOH refluxed 2 hrs. yielded 1.1 g. 3-amino-5-phenylpyrazole, m. 126-7.degree. (AcOEt-ligicoine or aq. MeOH).

1772-25-4, 1,3,6-Hexametricarbonitrile (prepn. of)

1772-25-4 CAPLUS

1,3,6-Hexametricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

ис— ch<sub>2</sub>— ch<sub>2</sub>— ch— (ch<sub>2</sub>)<sub>3</sub>— сn

L4 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2003 ACS ON STN
ACCESSION NUMBER: 1965:409759 CAPLUS
OCCUMENT NUMBER: 63:7959
ORIGINAL REFERENCE NO.: 63:1695c-d
TITLE: Electrolytic reductive coupling. VII. A new class of acrylonitrile oligomers
AUTHOR(S): Baizer, Manuel M.; Anderson, James D.
CORPORATE SOURCE: Monsanto Co., St. Louis, MO
SOURCE: CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal of Organic Chemistry (1965), 30(5), 1351-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Dournal English
AB Previous work on the electrolysis of acrylonitrile in aq.
quaternary ammonium salts under mildly alkaline conditions has been extended into the region of high acrylonitrile-water ratios. At very low water concns. acetone-soluble, relatively low-melting polyacrylonitriles of average mol. wt. 600-1300 are formed. From electrolysis of catholytes of intermediate (but still low) water content there were isolated an acrylonitrile hydro trimer,
1,3,6-tricyanohexane, and a mixt. of hydro tetramers, consisting of 1,3,6,8- and 1,3,5,8-tetracyanooctane. The structures of these new acrylonitrile oligomers were proved by conversion to and independent synthesis of the corresponding esters. The electrolytic hydropolymerization of acrylonitrile is viewed as proceeding from an initially formed .alpha., alpha.'-adiponitrile dianion.

IT IST2-42-5, 1,3,5,8-octaneterracarbonitrile is viewed as proceeding from an initially formed .alpha., alpha.'-adiponitrile dianion.

IT IST2-42-5, 1,3,5,8-octaneterracarbonitrile is viewed as proceeding from an initially formed .alpha., alpha.'-adiponitrile dianion.

IT IST2-42-5, 1,3,5,8-octaneterracarbonitrile is viewed as proceeding (prepn. of)

RN 1572-42-5 CAPLUS (prepn. of) 1572-42-5 CAPLUS 1,3,5,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

1572-43-6 CAPLUS
1,3,6,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

- CH2- CH2- CH2- CH2- CH2- CH2- CH2- CH

1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH-(CH2)3-CN

L4 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1965:409760 CAPLUS
DOCUMENT NUMBER: 63:9760
ORIGINAL REFERENCE NO.: 63:1695d-e
ITITLE: Electrolytic reductive coupling. VIII. Utilization and new preparation of .alpha.-methyleneglutaronitrile Baizer, Manuel M.; Anderson, James D. Monsanto Co., St. Louis, Mo Journal of Organic Chemistry (1965), 30(5), 1357-60 CODEN: JOCEAH; ISSN: 0022-3263 Journal English AUTHOR(S): CORPORATE SOURCE: SOURCE: SOURCE:

COEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
LANGUAGE: English

AB .alpha.-Methyleneglutaronitrile (I) has been electrolytically
hydrodimerized to yield | 1,3,6,8-tetracyanooctane (II). Electrolysis of a
mixture of I and acrylonitrile yielded II and adiponitrile-the
two hydro dimers-and | 1,3,6-tricyanohexane, the product of mixed coupling.
I and higher oligomers of acrylonitrile have been prepared by
the reaction of acrylonitrile with catalytic quantities of
tertiary phosphines in the presence of proton donors.

1 i572-42-5, | 1,3,5,8-Octanetetracarbonitrile 1572-43-6,
| 1,3,6,8-Octanetetracarbonitrile 1772-25-4, | 1,3,6Hexanetricarbonitrile
(prepn. of)

RN 1572-42-5 CAPLUS

CN 1,3,5,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

1572-43-6 CAPLUS 1,3,6,8-Octanetetracarbonitrile (7CI, 8CI) (CA INDEX NAME)

NC-CH2-CH2-CH-CH2-CH2-CH-CH2-CH2-CN

1772-25-4 CAPLUS
1,3,6-Hexanetricarbonitrile (7CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH2-CH2-CH- (CH2) 3-CN

L4 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN ACCESSION NUMBER: 1964: 425859 CAPLUS COCUMENT NUMBER: 61:25859 GRIGINAL REFERENCE NO.: 61:4507d-e 61:450/d-e
Coloration in acrylonitrile polymers
Takata, Toshihiro; Hiroi, Iwao: Taniyama, Masakazu
Toho Rayon Co. Ltd., Tokushima, Japan
Journal of Polymer Science, Part A: General Papers
(1964). 2(4), 1567-8
CODEN: JPYRAK: ISSN: 0449-2951 TITLE: AUTHOR(S): CORPORATE SOURCE: formed which supported the postulate of Grassie, et al. (G. and McNeill, CA 54, 16143a) for alkali-treated I. The intramol. ring closure leading to a similar structure for heat-treated I, as proposed by leading to a binum

Grassie,
et al., was also supported.

IT 64000-65-8, 2,4,6,8-Nonanetetracarbonitrile
(reaction with alc. KOH as model for discoloration of
acrylonitrile polymers)

RN 64000-86-8 CAPLUS
CN 2,4,6,8-Nonanetetracarbonitrile (7CI, 9CI) (CA INDEX NAME) 

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L4 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1961:130746 CAPLUS
DOCUMENT NUMBER: 55:130746
ORIGINAL REFERENCE NO: 55:24550b-d
TITLE: Synthesis of 1,3,5,7-tetracyanoheptane
AUTHOR(S): Vosburgh, W. C.; Green, D. L.
CORPORATE SOURCE: E. I. du Pont de Nemours and Co., Inc., Wilmington,
                                                                       Journal of Organic Chemistry (1961), 26, 2118-19
CODEN: JOCEAH; ISSN: 0022-3263
Journal
 DOCUMENT TYPE:
DOCUMENT FIFE.

Unavailable

AB 1,3,5,7-Tetracyanoheptane (I) was synthesized as a short-chain model for the polyacrylonitrile mol. HCHO was added to cyanoacetic ester (II) to give di-Et.alpha.,alpha.'-dicyanoglutarate (III): however, when the reaction temp. was not controlled, only Et.alpha.-cyanoacrylate was formed and it immediately polymerized to a low-mol.-wt. sticky polymer. Paraformaldehyde (60 g.) in 270 g. II treated during 4 hrs. with 4 ml.
              KOH in alc., after an addnl. 2 hrs. heating the mixt. adjusted to pH 4, and distd. gave 206 g. III, b0.4-0.6 150.5-1.5.degree., n240 1.4500, d24 1.416. III (180 g.), 300 ml. dioxane, and 102 ml. acrylontarile treated with 38.5 g. Triton B over 1 hr. at 30-5.degree., the soln. stirred 16 hrs., poured into R20, acidified, and extd. gave 160 g. 1,3,5,7-tetracyano-3,5-di-carbethoxyheptane (IV). Crude IV (160 g.)
mixed
              in 0.5 hr. with 84 g. KOH in 600 ml. MeOH and 400 ml. alc., the salt sepd., and washed gave 39 g. K.alpha., alpha.'-dicyano-.alpha., alpha.'-bis(.beta.-cyanoethyl)glutarate (V), m. 198-206.degree. (decompn.). V
 (30
              g.) in 250 ml. AcOH kept 2.5 hrs. at 90-100.degree., evapd., the residue extd. with CH2Cl2, dried, and evapd. gave 4.5 g. I, m. 106-7.degree.
               (MeOH).
100725-15-3, Glutaric acid, 2,4-dicyano-2,4-bis(2-cyanoethyl)-
ΙT
              (and derivs.)
100725-15-3 CAPLUS
Glutaric acid, 2,4-dicyano-2,4-bis(2-cyanoethyl)- (6CI) (CA INDEX NAME)
NC-CH2-CH2-
                                     с— сн<sub>2</sub>—
                                                         C-CH2-CH2-CN
             64918-24-7, 1,3,5,7-Heptanetetracarbonitrile
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1,3,5,7-Heptanetetracarbonitrile (6CI, 9CI) (CA INDEX NAME)

(prepn. of) 64918-24-7 CAPLUS

L4 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1959:77452 CAPLUS
DOCUMENT NUMBER: 53:77452
ORIGINAL REFERENCE NO. 53:13993c-i, 13994a-f
Oligomers. XIII. The oligomers of
acrylonitrile. 1. Syntheses
AUTHOR(S): Zahn, Helmut; Schafer, Paul
CORPORATE SOURCE: Univ. Heidelberg, Germany
COBN: CHBERM: ISSN: 0009-2940
DOCUMENT TYPE: Univ. Heidelberg, ISSN: 0009-2940
DOCUMENT TYPE: Unavailable
AB cf. C.A. 53, 13047c. Mech(CN)(COZET (30 g.) in 50 g. Me3COH treated
dropwise with 13 g. CH2:CHCN after the addn. of 0.75 cc. 301 KoH in MeOH,
the mixt. stirred 3 hrs. at 35.degree., neutralized with 2N HCl, dild.
with 400 cc. H20, extd. with Et20, and the ext. distd. gave 22 g.
MeC(CN)(COZET)(MYCCHZCN (I), b0.1 114-16.degree. I (9 g.) and 100 cc. HBr refluxed 8 hrs., evapd. in vacuo, the residue dissolved in H2O, extd. with Et2O, and the ext. dried and evapd. gave 6 g. HOZCCHMe(CH2)2CO2H, m. 77.degree. (C6H6). I (20 g.) in 40 cc. refluxing EtOH treated dropwise with 6.2 g. KOH in 30 cc. EtOH, the mixt. filtered, the residue washed with abs. EtOH, the residual salt dried (18 g.) dissolved in a little

the soln. treated with an equiv. amt. of concd. HCl, extd. with Et2O, and the ext. dried and evapd. left 13 g. oily, very hygroscopic
HOZCCME(CN) CHZCHZCN (II). II (12 g.) in 50 cc. C5H5N and 3 g. Cu powder refluxed 1 hr. at 110.degree., cooled, filtered, the C5H5N removed in vacuo, the residue treated with N HCl, extd. with EtOAc, and the ext. worked up yielded 6 g. McCH(CN)(CHZCHZCN, bl2 135.degree., n25) 1.4312. CHZ(COZEt)2 (116 g.), 2 g. Na, 30 cc. abs. EtOH and 73 g. CHZ:CMCCOZMe in 500 cc. dry Et2O refluxed 5 hrs., cooled, washed with 12 cc. AcOH in 120 cc. H2O, then with H2O, dried, and worked up yielded 140 g. McCCCCHMCCHZCHC(COZEt)2 (III), bl1 155-60.degree.. III (138 g.) in 230 g. Me3COCCHMCCHZCH (COZEt)2 (III), bl1 155-60.degree.. TII (139 g.) in 230 g. Me3COX treated with 10-15 drops CHZ:CHCN from a 29-g. portion and then with 1 cc. 30% KOH-MeOH at 35.degree., the remainder of the CHZ:CHCN d

while twice 1 cc. KOH-MeOH was added, stirred 2 hrs. at 30.degree., neutralized with 2N HCl, and poured into 1 l. H2O, and the crude product recrystd. from petr. ether yielded 148 g. Meo2CcHMecH2C(COZEL)2CH2CH2CN (IV), needles, m. 42.degree. IV (55 g.) in 150 cc. concd. HCl refluxed

hrs., treated with 50 cc. concd. HCl, refluxed 6 hrs., kept overnight, filtered from NH4Cl, treated 2-3 times with HCl, again filtered, the filtrate evapd. in vacuo, the oily residue dried over HZ504 and KOH, and the solid residue powdered and extd. in a Soxhlet app. with Bt20 yielded 37.5 g. HO2CCHMCCH2CH4(CO2H)CH2CH2CO2H (V), m. 95.degree. (Me2CO and CHCl3). V (1.5 g.) heated at 150.degree./12 mm. and the sublimate resublimed yielded 0.7 g. cyclic anhydride of V, needles, m. 82.degree. V (15 g.) in 30 cc. Ac20 refluxed 6 hrs., evapd. up to 180.degree., ed

ed at 210.degree./12 mm., and distd. gave 5 g. 3-methyl-4-oxocycloexane-carboxylic acid, b0.1 128-30.degree., m. 94.degree.. V (20 g.) in 100

concd. NH4OH evapd. on the water bath in vacuo left 23 g. NH4 salt of V. The NH4 salt (20 g.) in H2O treated with 46 g. AgNO3 in H2O pptd. the amorphous Ag salt of V, decomp. 205.degree.. Dry Br  $\{9$  cc. $\}$  in 46 cc.

CC14 treated with 30 g. Ag salt of V at 50.degree. in small portions, refluxed 0.5 hr., filtered, and the filtrate shaken with aq. satd.  $\sim$ 

L4 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Contin and 10% ag. KoH contg. NaCl, dried, and distd. yielded 6 g. alpha.-methyl-.gamma.-bromoethyl-.gamma.-butyrolactone, b0.01 (Continued)

egree...
V (12 g.), 48 cc. abs. EtOH, and 1 cc. concd. H2504 refluxed 7 hrs. gave 12 g. tri-Et ester of V, b0.07 110-15.degree... V (15 g.), 45 cc. abs. MeOH, and 1.2 concd. HCl gave similarly 13 g. tri-Me ester (VI) b0.02 98-101.degree... VI (40 g.) and 32 cc. liquid NH3 kept 4 weeks at root temp. In a sealed tube yielded 32.5 g. triamide (VII) of V, needles, m. 169.degree. (Me2CO). VII (10 g.) and 10 cc. POCl3 heated with stirring

70.degree., cooled, dissolved in iced H2O, neutralized with Na2CO3

with EtOAc, and the ext. distd. gave 1.0 g. NCCH2CH2CH(CN)CH2CH(CN)Me, b0.01 80.degree. (bath), n25D 1.4646. NCCH2COZET (VIII) (56.6 g.) in 100 g. dioxane treated dropwise with 53 g. CH2:CHCN while 4.5 cc. 30 KCH—MeOH was added in 4 portions, stirred 2 hrs. at room temp., neutralized with

HCl, and poured into 1 l. H2O yielded 105 g. Et ester (IX), prisms m. 37.degree., of HOZC(NC)C(CHZCHZCN)2 (X). IX (50 g.) in 150 cc. EtOH treated dropwise with 12.7 g. KOH in 50 cc. EtOH below 50.degree., filtered, and the residual salt washed with EtOH, dried in vacuo (48 g.), dissolved in a little H2O, acidfied with concd. HCl, and extd. with Et2O yielded 31 g. very hygroscopic X, m. 84.degree.. X (7 g.) in 40 cc.

refluxed with stirring during 45 min. at 110.degree. with 2 g. Cu powder, cooled, filtered, evapd. in vacuo, the residue treated with a little N HCl, extd. with EtoAc, and the ext. worked up yielded 2.2 g. NCCH(CHZCHZCN)2, b0.01 83.degree. (bath), n25D 1.4644. VIII (100 g.) and 30 g. 40% aq. CH2C treated with cooling and shaking with 0.6 cc. piperidine, refrigerated 2 hrs., kept at room temp. overnight, refluxed

hrs., neutralized with dil. HCl, and the product sepd., dried, and distd. yielded 51 g. CH2[CH(CN)CO2EL]2 (XI), b0.07 145-50.degree. VIII (57 g.) and 11.5 g. Na in 350 cc. refluxing abs. EtOH treated dropwise with stirring with 60 g. CH2Br2, stirred 3 hrs. at room temp. refluxed 4 hrs., kept overnight, filtered, concd., poured into H2O, neutralized with dil. HCl, and extd. with Et2O yielded XI. XI (47 g.) in 100 cc. Me3COH treated

HCL, and extd. with EtZO yielded XI. XI (47 g.) in 100 cc. Me3COH ted dropwise with stirring at reflux with 21 g. CH2:CHCN, while three 1-cc. portions 30% KOH-MeOH were added, stirred 3 hrs. at room temp., neutralized with 2N HCl, poured into 1 l. HZO, and worked up in the usual manner yielded 32 g. CH2[c(CN) (COZEY.CHZCHZON]2 (XII), needles, m. 95. degree. (EtOH). XII (30 g.) in 100 cc. refluxing EtOH treated with stirring dropwise with 9.7 g. KOH in 30 cc. EtOH, kept overnight, filtered, and the solid washed, dried, acidified with concd. HCl, and extd. with EtZO yielded 13 g. CHZ[c(CN) (COZEY.CHZCN]2 (XIII), very hygroscopic, m. 136.degree. XIII (5 g.) in 50 cc. CSHSN refluxed 1.5 hrs. at 110.degree. with stirring with 3 g. Cu, cooled, filtered, evapd. in vacuo, the residue treated with a little N HCl, extd. with EtOA, and the ext. worked up yielded 0.5 g. CH2[C(RN) CECEXCN]2, bo. 01 95.degree. (bath). CH2[CH(COZEY.12]2 (30 g.) in 50 cc. refluxing dioxane treated dropwise with stirring with 10 g. CH2:CECN, and the mixt. treated in the usual manner at the beginning and the end of the addin. with 1 cc. 30% (KOH-MeON, and then processed gave 18 g. CHZ[c(COZEY.2CHZCN]2].

ANSWER 38 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN (Continued), Glutaric acid, 2,4-dicyano-2,4-bis(2-cyanoethyl)- 107273-45-0, Glutaric acid, 2,0-dicyano-2,4-bis(2-cyanoethyl)-, diethyl ester (prepn. of) 64918-24-7 CAPLUS 1,3,5,7-Heptanetetracarbonitrile (6CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{CN} & \mathsf{CN} \\ | & | \\ \mathsf{NC-CH}_2 - \mathsf{CH}_2 - \mathsf{CH-CH}_2 - \mathsf{CH-CH}_2 - \mathsf{CH}_2 - \mathsf{CN} \end{array}$$

100725-15-3 CAPLUS Glutaric acid, 2,4-dicyano-2,4-bis(2-cyanoethyl)- (6CI) (CA INDEX NAME)

107273-45-0 CAPLUS Glutaric acid, 2,4-dicyano-2,4-bis(2-cyanoethyl)-, diethyl ester (6CI) (CA INDEX NAME)

ACCESSION NUMBER: 1955:59012 CAPLUS
DOCUMENT NUMBER: 49:59012 CAPLUS
ORIGINAL REFFRENCE NO.: 49:11363b-d
TITLE: The properties of nitrile binary systems and their relation to polyacrylonitrile solubility
AUTHOR(S): Phibbs, M. K.
CORPORATE SOURCE: Dupont Co. Can., Kingston, ON
SOURCE: Journal of Physical Chemistry (1955), 59, 346-53
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The solvent powers of liquids for 1,3,5,7-tetracyanoheptane and for polyacrylonitrile are qualitatively the same. Good nitrile solvents are characterized by heat evolution and vol. expansion on mixing with glutaronitrile. A qual. correlation exists between excess entropies of mixing and nonideal vol. changes on mixing in the nitrile binary systems. Vapor pressure and viscosity data are given for some glutaronitrile binary systems. No correlation exists between viscosity and any of the other measured properties. Good nitrile solvents must be composed of mols. high dipole moments, a low hydrocarbon/polar group ratio, and no self.H-bonding power.
64918-247-7, 1, 3, 5, 7-Heptanetetracarbonitrile
(soly. of)
64918-247-7 CAPLUS
1,3,5,7-Heptanetetracarbonitrile (6CI, 9CI) (CA INDEX NAME)

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